

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Diaqua{ μ_2 -*N,N'*-bis[(cyclohexanylidene)-amino]oxamide}bis(triphenylphosphane)-silver(I) dinitrate

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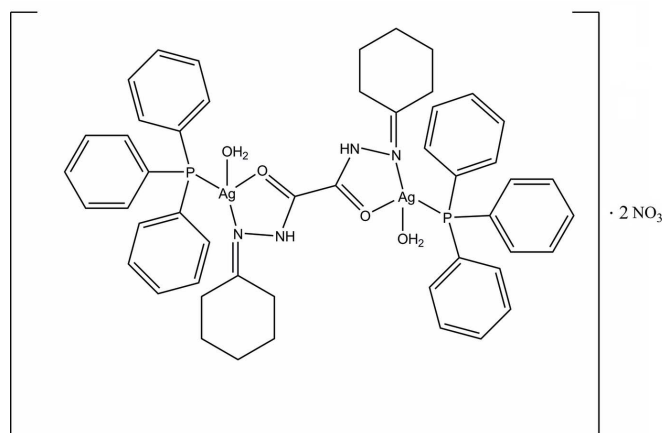
Received 17 December 2013; accepted 22 December 2013

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.028; wR factor = 0.072; data-to-parameter ratio = 24.3.

The dinuclear title compound, $[\text{Ag}_2(\text{C}_{14}\text{H}_{22}\text{N}_4\text{O}_2)(\text{C}_{18}\text{H}_{15}\text{P})_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$, lies across an inversion center and consists of two $[\text{Ag}(\text{H}_2\text{O})(\text{PPh}_3)]$ units bridged by a bis(cyclohexanone)-oxalydihydrazone ligand. The charge-balance is supplied by two nitrate anions. The symmetry-unique Ag^{I} ion is in a distorted tetrahedral geometry coordinated by a P atom from a triphenylphosphane ligand, an O atom from a water molecule and a bis(cyclohexanone)oxalydihydrazone ligand bidentate chelating through the O atom and one of N atoms. In the crystal, $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link the components, forming chains along the b -axis direction. These chains are connected through weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, leading to the formation of a two-dimensional supramolecular network parallel to (001).

Related literature

For potential applications of hydrazone derivatives, see: Fouda *et al.* (2007); Qu *et al.* (2011); van der Star *et al.* (2012). For the use of metal(I) complexes of phosphine ligands as precursors for the preparation of mixed-ligand complexes, see: Nawaz *et al.* (2011); Pakawatchai *et al.* (2012). For a related structure, see: Wattanakanjana *et al.* (2013).



Experimental

Crystal data

$[\text{Ag}_2(\text{C}_{14}\text{H}_{22}\text{N}_4\text{O}_2)(\text{C}_{18}\text{H}_{15}\text{P})_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$
 $M_r = 1178.68$
 Triclinic, $P\bar{1}$
 $a = 9.0903$ (8) Å
 $b = 9.5730$ (8) Å
 $c = 15.2638$ (13) Å
 $\alpha = 74.617$ (1)°

$\beta = 83.676$ (1)°
 $\gamma = 77.091$ (1)°
 $V = 1246.49$ (18) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.91$ mm⁻¹
 $T = 100$ K
 $0.42 \times 0.38 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2012)
 $T_{\text{min}} = 0.624$, $T_{\text{max}} = 0.746$

29613 measured reflections
 7621 independent reflections
 7076 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.072$
 $S = 1.02$
 7621 reflections

313 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.50$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.54$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{O}2-\text{H}2A\cdots\text{O}3$ | 0.80 | 2.02 | 2.8103 (17) | 167 |
| $\text{O}2-\text{H}2B\cdots\text{O}3^i$ | 0.88 | 1.98 | 2.8684 (16) | 177 |
| $\text{N}1-\text{H}1\cdots\text{O}5^i$ | 0.88 | 2.16 | 2.8407 (19) | 134 |
| $\text{C}22-\text{H}22\cdots\text{O}4$ | 0.95 | 2.58 | 3.297 (2) | 133 |

Symmetry code: (i) $-x + 1, -y + 1, -z$.

Data collection: APEX2 (Bruker, 2012); cell refinement: SAINT (Bruker, 2012); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2012 (Sheldrick, 2008), SHELXLE (Hübschle *et al.*, 2011); molecular graphics: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: SHELXL97 and publCIF (Westrip, 2010).

Financial support from the Center of Excellence for Innovation in Chemistry (PERCH-CIC), the Office of the Higher Education Commission, Ministry of Education, and the

Department of Chemistry, Prince of Songkla University, is gratefully acknowledged. RN would like to thank Dr Matthias Zeller for valuable suggestions and assistance with the X-ray structure determination and use of structure refinement programs.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5679).

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supporting information

Acta Cryst. (2014). E70, m30–m31 [doi:10.1107/S1600536813034454]

Diaqua $\{\mu_2$ -*N,N'*-bis[(cyclohexanylidene)amino]oxamide}bis(triphenylphosphane)silver(I) dinitrate

Ruthairat Nimthong, Nattakunya Thepsena, Walailak Puetpaiboon and Yupa Wattanakanjana

S1. Comment

Studies of hydrazone derivatives containing nitrogen and oxygen have recently attracted considerable attention because not only are they corrosion inhibitors but it has been discovered that they are effective in different types of media (Fouda *et al.*, 2007; Qu *et al.*, 2011). They are an invaluable tool for studying mechanisms of acquired demyelination and remyelination which are histological hallmarks of multiple sclerosis (MS) (van der Star *et al.*, 2012). Silver(I) complexes of phosphine ligands have been extensively studied as precursors for preparing mixed-ligand complexes having different geometries such as mononuclear and dinuclear (Nawaz *et al.*, 2011; Pakawatchai *et al.*, 2012). Here, we report the crystal structure of the title compound.

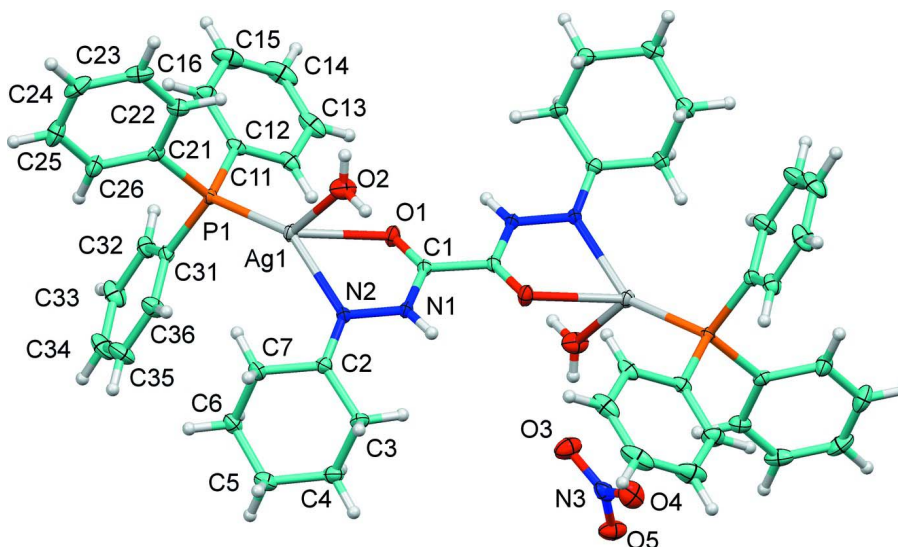
The molecular structure of the title compound is shown in Fig. 1. The symmetry unique Ag^I ion is coordinated to the P atom of a triphenylphosphane ligand and the O atom of water molecule which forms the [Ag(H₂O)(PPh₃)] units. The bis-(cyclohexanone)oxalyldihydrazone ligand, located on an inversion center, acts as a bidentate bridging ligand between the two [Ag(H₂O)(PPh₃)] units by way of one O atom and one N atom. The Ag^I ion displays a distorted tetrahedral coordination. The P1—Ag1 bond length of 2.3369 (4) Å is shorter than that found in for example [Ag₂C₁₂(CH₃N₃S)₂(C₁₈H₁₅P)₂], which is 2.4225 (4) Å (Wattanakanjana *et al.*, 2013). In the crystal, hydrogen bonds play a key role stabilizing a 2-D network. Intermolecular O—H \cdots O hydrogen bonds occur where the oxygen atoms of nitrate anions serve as acceptors while H atoms of water molecules act as donors (Table 1). In addition, a pair of O—H \cdots O hydrogen bonds form a four-membered O₂H₂ ring within a 1-D chain along [010] (Fig. 2). The chains are connected through weak C—H \cdots O hydrogen bonds leading to the formation of a 2-D supramolecular network parallel to (001) as shown in Figure 3.

S2. Experimental

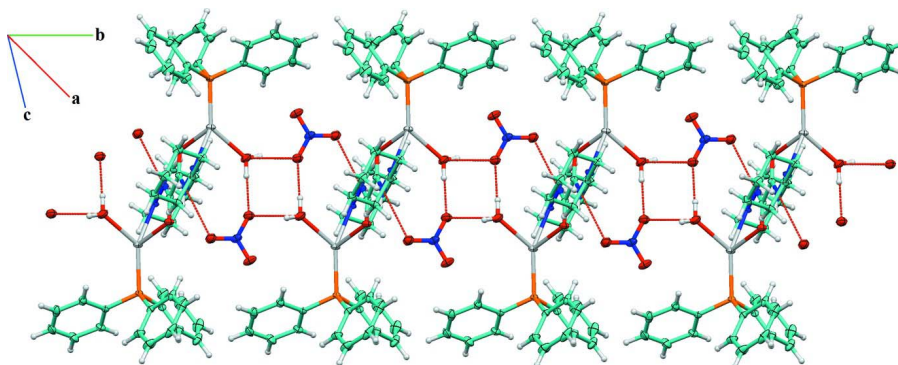
Bis(cyclohexanone)oxalyldihydrazone, BCO, (0.16g,0.58 mmol) was dissolved in 30 cm³ of methanol at 332 K. AgNO₃ (0.10g,0.59 mmol) was added and the mixture was stirred for 3 hours. Triphenylphosphine, PPh₃, (0.31g,1.18 mmol) was added and new reaction mixture was heated under reflux for 2 hours. The resulting clear solution was filtered off and left to evaporate at room temperature. Colorless crystals, which were deposited upon standing for 6 days, were filtered off and dried under reduced pressure.

S3. Refinement

H atoms bonded to C and N atoms were included in calculated positions with C—H = 0.95–0.99Å, N—H = 0.88Å and refined in a riding-model approximation with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C},\text{N})$. The H atoms of the water molecules were included 'as found' positions with $1.5U_{\text{eq}}(\text{O})$.

**Figure 1**

The molecular structure with displacement ellipsoids drawn at the 30% probability level. Only the symmetry unique anion is shown and the asymmetric unit labelled.

**Figure 2**

Part of the crystal structure of $[\{Ag(H_2O)(C_{18}H_{15}P)\}_2(C_{14}H_{22}N_4O_2)] \cdot (NO_3)_2$ with O—H \cdots O hydrogen bonds (red dashed lines) showing 1-D chain along [010] axis.

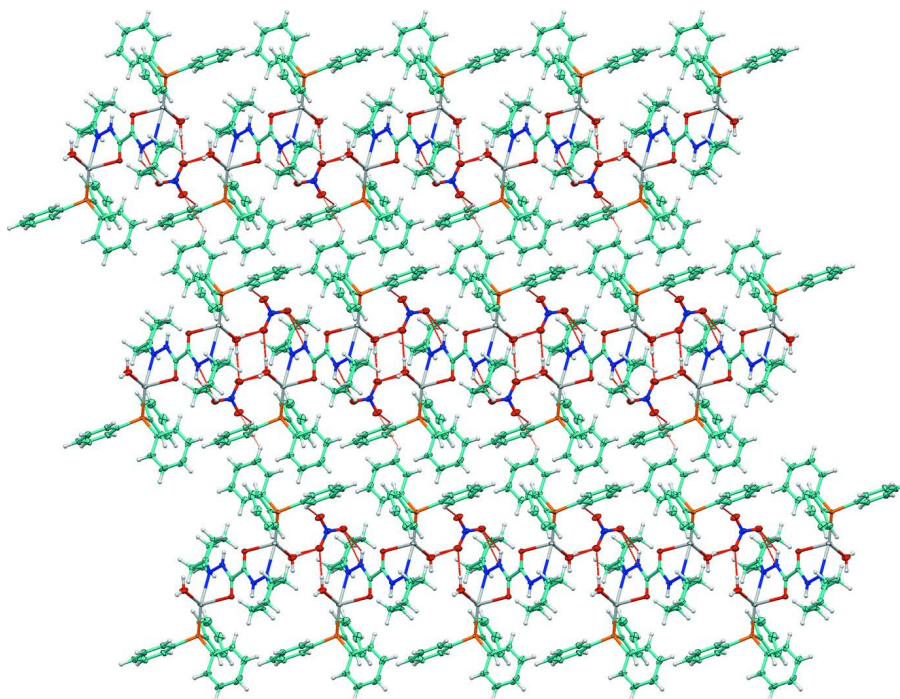


Figure 3

A Fragment of the 2-D network of $[\{\text{Ag}(\text{H}_2\text{O})(\text{C}_{18}\text{H}_{15}\text{P})_2(\text{C}_{14}\text{H}_{22}\text{N}_4\text{O}_2)\}](\text{NO}_3)_2$, showing C—H \cdots O hydrogen bonds viewed along the a axis.

Diaqua $\{\mu_2$ - N,N' -bis[(cyclohexanylidene)amino]oxamide}bis(triphenylphosphane)silver(I) dinitrate

Crystal data

$[\text{Ag}_2(\text{C}_{14}\text{H}_{22}\text{N}_4\text{O}_2)(\text{C}_{18}\text{H}_{15}\text{P})_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$

$M_r = 1178.68$

Triclinic, $P\bar{1}$

$a = 9.0903$ (8) Å

$b = 9.5730$ (8) Å

$c = 15.2638$ (13) Å

$\alpha = 74.617$ (1)°

$\beta = 83.676$ (1)°

$\gamma = 77.091$ (1)°

$V = 1246.49$ (18) Å³

$Z = 1$

$F(000) = 602$

$D_x = 1.570$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6878 reflections

$\theta = 2.3$ – 31.3 °

$\mu = 0.91$ mm⁻¹

$T = 100$ K

Plate, colourless

$0.42 \times 0.38 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: sealed tube

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2012)

$T_{\min} = 0.624$, $T_{\max} = 0.746$

29613 measured reflections

7621 independent reflections

7076 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

$\theta_{\max} = 31.6$ °, $\theta_{\min} = 2.3$ °

$h = -13 \rightarrow 13$

$k = -13 \rightarrow 13$

$l = -22 \rightarrow 22$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.028$ $wR(F^2) = 0.072$ $S = 1.02$

7621 reflections

313 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.444P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 1.50 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$ *Special details***Experimental.** Reflections 0 0 1 was affected by the beam stop and was omitted from the refinement.**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)*

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| Ag1 | 0.77397 (2) | 0.67531 (2) | 0.14033 (2) | 0.01512 (4) |
| P1 | 0.87389 (4) | 0.59821 (4) | 0.28403 (3) | 0.01204 (7) |
| O1 | 0.58233 (10) | 0.91020 (10) | 0.10413 (6) | 0.0182 (2) |
| O2 | 0.60176 (10) | 0.57786 (10) | 0.07530 (6) | 0.0278 (3) |
| H2A | 0.5453 | 0.5216 | 0.0951 | 0.042* |
| H2B | 0.5935 | 0.5990 | 0.0158 | 0.042* |
| O3 | 0.41980 (18) | 0.36454 (16) | 0.11758 (9) | 0.0311 (3) |
| O4 | 0.46973 (17) | 0.30464 (18) | 0.26020 (10) | 0.0327 (3) |
| O5 | 0.37588 (17) | 0.15741 (16) | 0.20689 (9) | 0.0289 (3) |
| N1 | 0.67258 (14) | 0.90320 (14) | -0.04115 (9) | 0.0146 (2) |
| H1 | 0.6597 | 0.9387 | -0.0998 | 0.017* |
| N2 | 0.80176 (14) | 0.79893 (14) | -0.00875 (9) | 0.0144 (2) |
| N3 | 0.42173 (16) | 0.27494 (17) | 0.19571 (10) | 0.0211 (3) |
| C1 | 0.56953 (16) | 0.94638 (16) | 0.02131 (10) | 0.0132 (3) |
| C2 | 0.91980 (17) | 0.79182 (17) | -0.06359 (10) | 0.0160 (3) |
| C3 | 0.93888 (19) | 0.88935 (19) | -0.15685 (11) | 0.0203 (3) |
| H3A | 0.8466 | 0.9672 | -0.1707 | 0.024* |
| H3B | 0.9540 | 0.8301 | -0.2025 | 0.024* |
| C4 | 1.0763 (2) | 0.96139 (19) | -0.16206 (12) | 0.0220 (3) |
| H4A | 1.0959 | 1.0152 | -0.2258 | 0.026* |
| H4B | 1.0528 | 1.0343 | -0.1245 | 0.026* |
| C5 | 1.21787 (19) | 0.8478 (2) | -0.12903 (12) | 0.0222 (3) |
| H5A | 1.2474 | 0.7802 | -0.1699 | 0.027* |
| H5B | 1.3020 | 0.8989 | -0.1309 | 0.027* |
| C6 | 1.19021 (19) | 0.75881 (19) | -0.03247 (12) | 0.0210 (3) |
| H6A | 1.1659 | 0.8255 | 0.0091 | 0.025* |
| H6B | 1.2827 | 0.6846 | -0.0123 | 0.025* |

| | | | | |
|-----|--------------|--------------|---------------|------------|
| C7 | 1.05827 (18) | 0.68022 (18) | -0.02872 (11) | 0.0185 (3) |
| H7A | 1.0861 | 0.6074 | -0.0663 | 0.022* |
| H7B | 1.0371 | 0.6264 | 0.0348 | 0.022* |
| C11 | 0.74414 (17) | 0.67524 (18) | 0.36679 (11) | 0.0163 (3) |
| C12 | 0.66381 (18) | 0.82024 (19) | 0.33780 (12) | 0.0204 (3) |
| H12 | 0.6780 | 0.8747 | 0.2768 | 0.024* |
| C13 | 0.5628 (2) | 0.8854 (2) | 0.39823 (15) | 0.0289 (4) |
| H13 | 0.5084 | 0.9842 | 0.3786 | 0.035* |
| C14 | 0.5425 (2) | 0.8049 (3) | 0.48700 (15) | 0.0347 (5) |
| H14 | 0.4741 | 0.8492 | 0.5284 | 0.042* |
| C15 | 0.6211 (2) | 0.6599 (3) | 0.51627 (14) | 0.0338 (4) |
| H15 | 0.6058 | 0.6054 | 0.5772 | 0.041* |
| C16 | 0.7224 (2) | 0.5946 (2) | 0.45616 (12) | 0.0244 (3) |
| H16 | 0.7765 | 0.4957 | 0.4759 | 0.029* |
| C21 | 0.91018 (18) | 0.39933 (16) | 0.33027 (10) | 0.0146 (3) |
| C22 | 0.7932 (2) | 0.32645 (19) | 0.32916 (11) | 0.0201 (3) |
| H22 | 0.6984 | 0.3814 | 0.3067 | 0.024* |
| C23 | 0.8160 (2) | 0.1736 (2) | 0.36097 (12) | 0.0262 (4) |
| H23 | 0.7362 | 0.1240 | 0.3613 | 0.031* |
| C24 | 0.9551 (3) | 0.0933 (2) | 0.39231 (13) | 0.0297 (4) |
| H24 | 0.9703 | -0.0113 | 0.4139 | 0.036* |
| C25 | 1.0718 (3) | 0.1643 (2) | 0.39229 (14) | 0.0309 (4) |
| H25 | 1.1671 | 0.1084 | 0.4132 | 0.037* |
| C26 | 1.0499 (2) | 0.31784 (19) | 0.36159 (12) | 0.0222 (3) |
| H26 | 1.1299 | 0.3667 | 0.3620 | 0.027* |
| C31 | 1.05027 (17) | 0.65300 (16) | 0.29052 (11) | 0.0152 (3) |
| C32 | 1.07908 (19) | 0.70550 (18) | 0.36258 (12) | 0.0204 (3) |
| H32 | 1.0065 | 0.7101 | 0.4120 | 0.025* |
| C33 | 1.2145 (2) | 0.7513 (2) | 0.36192 (15) | 0.0296 (4) |
| H33 | 1.2338 | 0.7877 | 0.4108 | 0.036* |
| C34 | 1.3209 (2) | 0.7438 (2) | 0.29016 (16) | 0.0337 (4) |
| H34 | 1.4121 | 0.7769 | 0.2895 | 0.040* |
| C35 | 1.2953 (2) | 0.6887 (3) | 0.21933 (15) | 0.0322 (4) |
| H35 | 1.3696 | 0.6816 | 0.1709 | 0.039* |
| C36 | 1.1601 (2) | 0.6437 (2) | 0.21948 (13) | 0.0243 (3) |
| H36 | 1.1421 | 0.6062 | 0.1708 | 0.029* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|---------------|---------------|
| Ag1 | 0.01432 (6) | 0.01811 (6) | 0.01070 (6) | 0.00005 (4) | -0.00308 (4) | -0.00155 (4) |
| P1 | 0.01111 (16) | 0.01418 (16) | 0.01055 (16) | -0.00195 (13) | -0.00170 (12) | -0.00267 (13) |
| O1 | 0.0195 (5) | 0.0194 (5) | 0.0129 (5) | 0.0032 (4) | -0.0034 (4) | -0.0040 (4) |
| O2 | 0.0328 (7) | 0.0370 (7) | 0.0208 (6) | -0.0188 (6) | -0.0022 (5) | -0.0096 (5) |
| O3 | 0.0411 (8) | 0.0359 (7) | 0.0194 (6) | -0.0171 (6) | -0.0039 (6) | -0.0038 (5) |
| O4 | 0.0329 (7) | 0.0479 (9) | 0.0250 (7) | -0.0109 (6) | -0.0062 (6) | -0.0180 (6) |
| O5 | 0.0355 (7) | 0.0358 (7) | 0.0203 (6) | -0.0179 (6) | 0.0022 (5) | -0.0078 (5) |
| N1 | 0.0128 (6) | 0.0159 (6) | 0.0118 (5) | 0.0001 (5) | -0.0018 (4) | 0.0000 (5) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|-------------|--------------|
| N2 | 0.0106 (5) | 0.0161 (6) | 0.0137 (6) | 0.0000 (4) | -0.0011 (4) | -0.0010 (5) |
| N3 | 0.0161 (6) | 0.0308 (7) | 0.0187 (6) | -0.0047 (6) | 0.0005 (5) | -0.0107 (6) |
| C1 | 0.0121 (6) | 0.0127 (6) | 0.0146 (6) | -0.0020 (5) | -0.0030 (5) | -0.0023 (5) |
| C2 | 0.0140 (7) | 0.0186 (7) | 0.0151 (7) | -0.0040 (5) | -0.0003 (5) | -0.0034 (5) |
| C3 | 0.0171 (7) | 0.0265 (8) | 0.0140 (7) | -0.0055 (6) | 0.0016 (5) | 0.0005 (6) |
| C4 | 0.0216 (8) | 0.0230 (8) | 0.0205 (8) | -0.0075 (6) | 0.0036 (6) | -0.0033 (6) |
| C5 | 0.0177 (7) | 0.0277 (8) | 0.0237 (8) | -0.0084 (6) | 0.0026 (6) | -0.0092 (7) |
| C6 | 0.0151 (7) | 0.0267 (8) | 0.0219 (8) | -0.0028 (6) | -0.0003 (6) | -0.0088 (6) |
| C7 | 0.0139 (7) | 0.0193 (7) | 0.0203 (7) | -0.0008 (6) | -0.0003 (6) | -0.0041 (6) |
| C11 | 0.0124 (6) | 0.0231 (7) | 0.0168 (7) | -0.0053 (6) | 0.0005 (5) | -0.0095 (6) |
| C12 | 0.0148 (7) | 0.0222 (7) | 0.0286 (8) | -0.0055 (6) | 0.0001 (6) | -0.0131 (7) |
| C13 | 0.0178 (8) | 0.0323 (9) | 0.0458 (11) | -0.0070 (7) | 0.0044 (7) | -0.0266 (9) |
| C14 | 0.0253 (9) | 0.0514 (12) | 0.0426 (11) | -0.0163 (9) | 0.0126 (8) | -0.0367 (10) |
| C15 | 0.0325 (10) | 0.0552 (13) | 0.0228 (9) | -0.0190 (9) | 0.0096 (7) | -0.0213 (9) |
| C16 | 0.0246 (8) | 0.0339 (9) | 0.0160 (7) | -0.0081 (7) | 0.0016 (6) | -0.0079 (7) |
| C21 | 0.0181 (7) | 0.0148 (6) | 0.0109 (6) | -0.0044 (5) | -0.0003 (5) | -0.0022 (5) |
| C22 | 0.0209 (8) | 0.0215 (7) | 0.0201 (7) | -0.0086 (6) | 0.0028 (6) | -0.0069 (6) |
| C23 | 0.0357 (10) | 0.0241 (8) | 0.0231 (8) | -0.0164 (7) | 0.0103 (7) | -0.0094 (7) |
| C24 | 0.0493 (12) | 0.0160 (7) | 0.0212 (8) | -0.0078 (8) | 0.0020 (8) | -0.0008 (6) |
| C25 | 0.0383 (11) | 0.0196 (8) | 0.0289 (9) | 0.0019 (7) | -0.0101 (8) | 0.0010 (7) |
| C26 | 0.0249 (8) | 0.0183 (7) | 0.0213 (8) | -0.0020 (6) | -0.0074 (6) | -0.0005 (6) |
| C31 | 0.0128 (6) | 0.0141 (6) | 0.0180 (7) | -0.0027 (5) | -0.0029 (5) | -0.0021 (5) |
| C32 | 0.0175 (7) | 0.0209 (7) | 0.0248 (8) | -0.0042 (6) | -0.0044 (6) | -0.0073 (6) |
| C33 | 0.0219 (8) | 0.0336 (10) | 0.0408 (11) | -0.0080 (7) | -0.0083 (8) | -0.0173 (8) |
| C34 | 0.0171 (8) | 0.0388 (11) | 0.0508 (13) | -0.0101 (8) | -0.0037 (8) | -0.0163 (9) |
| C35 | 0.0167 (8) | 0.0450 (11) | 0.0377 (11) | -0.0099 (8) | 0.0055 (7) | -0.0147 (9) |
| C36 | 0.0175 (8) | 0.0337 (9) | 0.0253 (8) | -0.0082 (7) | 0.0026 (6) | -0.0123 (7) |

Geometric parameters (Å, °)

| | | | |
|--------------------|-------------|---------|-----------|
| Ag1—N2 | 2.2849 (13) | C11—C16 | 1.395 (2) |
| Ag1—P1 | 2.3369 (4) | C11—C12 | 1.396 (2) |
| Ag1—O2 | 2.4068 | C12—C13 | 1.395 (2) |
| Ag1—O1 | 2.4898 (9) | C12—H12 | 0.9500 |
| P1—C21 | 1.8137 (15) | C13—C14 | 1.385 (3) |
| P1—C31 | 1.8149 (16) | C13—H13 | 0.9500 |
| P1—C11 | 1.8187 (16) | C14—C15 | 1.391 (3) |
| O1—C1 | 1.2304 (17) | C14—H14 | 0.9500 |
| O2—H2A | 0.8048 | C15—C16 | 1.393 (3) |
| O2—H2B | 0.8848 | C15—H15 | 0.9500 |
| O3—N3 | 1.270 (2) | C16—H16 | 0.9500 |
| O4—N3 | 1.2404 (19) | C21—C26 | 1.394 (2) |
| O5—N3 | 1.249 (2) | C21—C22 | 1.400 (2) |
| N1—C1 | 1.340 (2) | C22—C23 | 1.389 (2) |
| N1—N2 | 1.4008 (17) | C22—H22 | 0.9500 |
| N1—H1 | 0.8800 | C23—C24 | 1.387 (3) |
| N2—C2 | 1.287 (2) | C23—H23 | 0.9500 |
| C1—C1 ⁱ | 1.524 (3) | C24—C25 | 1.382 (3) |

| | | | |
|-----------------------|-------------|-------------|-------------|
| C2—C3 | 1.497 (2) | C24—H24 | 0.9500 |
| C2—C7 | 1.501 (2) | C25—C26 | 1.394 (2) |
| C3—C4 | 1.542 (2) | C25—H25 | 0.9500 |
| C3—H3A | 0.9900 | C26—H26 | 0.9500 |
| C3—H3B | 0.9900 | C31—C32 | 1.395 (2) |
| C4—C5 | 1.523 (2) | C31—C36 | 1.398 (2) |
| C4—H4A | 0.9900 | C32—C33 | 1.394 (2) |
| C4—H4B | 0.9900 | C32—H32 | 0.9500 |
| C5—C6 | 1.519 (2) | C33—C34 | 1.385 (3) |
| C5—H5A | 0.9900 | C33—H33 | 0.9500 |
| C5—H5B | 0.9900 | C34—C35 | 1.384 (3) |
| C6—C7 | 1.541 (2) | C34—H34 | 0.9500 |
| C6—H6A | 0.9900 | C35—C36 | 1.390 (3) |
| C6—H6B | 0.9900 | C35—H35 | 0.9500 |
| C7—H7A | 0.9900 | C36—H36 | 0.9500 |
| C7—H7B | 0.9900 | | |
| N2—Ag1—P1 | 146.83 (3) | C2—C7—H7B | 109.7 |
| N2—Ag1—O2 | 80.48 (4) | C6—C7—H7B | 109.7 |
| P1—Ag1—O2 | 130.70 (2) | H7A—C7—H7B | 108.2 |
| N2—Ag1—O1 | 69.04 (4) | C16—C11—C12 | 120.00 (15) |
| P1—Ag1—O1 | 118.43 (2) | C16—C11—P1 | 122.44 (13) |
| O2—Ag1—O1 | 84.40 (3) | C12—C11—P1 | 117.56 (12) |
| C21—P1—C31 | 105.26 (7) | C13—C12—C11 | 120.17 (17) |
| C21—P1—C11 | 105.67 (7) | C13—C12—H12 | 119.9 |
| C31—P1—C11 | 104.89 (7) | C11—C12—H12 | 119.9 |
| C21—P1—Ag1 | 113.89 (5) | C14—C13—C12 | 119.49 (19) |
| C31—P1—Ag1 | 115.29 (5) | C14—C13—H13 | 120.3 |
| C11—P1—Ag1 | 110.99 (5) | C12—C13—H13 | 120.3 |
| C1—O1—Ag1 | 107.71 (8) | C13—C14—C15 | 120.72 (17) |
| Ag1—O2—H2A | 135.1 | C13—C14—H14 | 119.6 |
| Ag1—O2—H2B | 121.5 | C15—C14—H14 | 119.6 |
| H2A—O2—H2B | 103.3 | C14—C15—C16 | 119.94 (19) |
| C1—N1—N2 | 116.91 (12) | C14—C15—H15 | 120.0 |
| C1—N1—H1 | 121.5 | C16—C15—H15 | 120.0 |
| N2—N1—H1 | 121.5 | C15—C16—C11 | 119.67 (19) |
| C2—N2—N1 | 117.05 (13) | C15—C16—H16 | 120.2 |
| C2—N2—Ag1 | 129.26 (11) | C11—C16—H16 | 120.2 |
| N1—N2—Ag1 | 113.55 (9) | C26—C21—C22 | 119.82 (15) |
| O4—N3—O5 | 120.55 (16) | C26—C21—P1 | 122.88 (12) |
| O4—N3—O3 | 119.69 (16) | C22—C21—P1 | 117.21 (12) |
| O5—N3—O3 | 119.76 (14) | C23—C22—C21 | 119.81 (17) |
| O1—C1—N1 | 125.99 (13) | C23—C22—H22 | 120.1 |
| O1—C1—C1 ⁱ | 121.54 (17) | C21—C22—H22 | 120.1 |
| N1—C1—C1 ⁱ | 112.43 (16) | C24—C23—C22 | 120.06 (17) |
| N2—C2—C3 | 127.37 (15) | C24—C23—H23 | 120.0 |
| N2—C2—C7 | 117.00 (14) | C22—C23—H23 | 120.0 |
| C3—C2—C7 | 115.50 (13) | C25—C24—C23 | 120.41 (16) |

| | | | |
|---------------------------|--------------|-----------------|--------------|
| C2—C3—C4 | 109.85 (14) | C25—C24—H24 | 119.8 |
| C2—C3—H3A | 109.7 | C23—C24—H24 | 119.8 |
| C4—C3—H3A | 109.7 | C24—C25—C26 | 120.14 (18) |
| C2—C3—H3B | 109.7 | C24—C25—H25 | 119.9 |
| C4—C3—H3B | 109.7 | C26—C25—H25 | 119.9 |
| H3A—C3—H3B | 108.2 | C21—C26—C25 | 119.75 (17) |
| C5—C4—C3 | 112.15 (14) | C21—C26—H26 | 120.1 |
| C5—C4—H4A | 109.2 | C25—C26—H26 | 120.1 |
| C3—C4—H4A | 109.2 | C32—C31—C36 | 119.17 (15) |
| C5—C4—H4B | 109.2 | C32—C31—P1 | 122.66 (12) |
| C3—C4—H4B | 109.2 | C36—C31—P1 | 118.16 (12) |
| H4A—C4—H4B | 107.9 | C33—C32—C31 | 119.95 (17) |
| C6—C5—C4 | 110.70 (14) | C33—C32—H32 | 120.0 |
| C6—C5—H5A | 109.5 | C31—C32—H32 | 120.0 |
| C4—C5—H5A | 109.5 | C34—C33—C32 | 120.11 (18) |
| C6—C5—H5B | 109.5 | C34—C33—H33 | 119.9 |
| C4—C5—H5B | 109.5 | C32—C33—H33 | 119.9 |
| H5A—C5—H5B | 108.1 | C35—C34—C33 | 120.54 (17) |
| C5—C6—C7 | 109.82 (14) | C35—C34—H34 | 119.7 |
| C5—C6—H6A | 109.7 | C33—C34—H34 | 119.7 |
| C7—C6—H6A | 109.7 | C34—C35—C36 | 119.52 (18) |
| C5—C6—H6B | 109.7 | C34—C35—H35 | 120.2 |
| C7—C6—H6B | 109.7 | C36—C35—H35 | 120.2 |
| H6A—C6—H6B | 108.2 | C35—C36—C31 | 120.69 (17) |
| C2—C7—C6 | 109.86 (13) | C35—C36—H36 | 119.7 |
| C2—C7—H7A | 109.7 | C31—C36—H36 | 119.7 |
| C6—C7—H7A | 109.7 | | |
| | | | |
| C1—N1—N2—C2 | -158.29 (14) | C12—C11—C16—C15 | -0.4 (3) |
| C1—N1—N2—Ag1 | 17.79 (16) | P1—C11—C16—C15 | -179.89 (14) |
| Ag1—O1—C1—N1 | -22.20 (17) | C31—P1—C21—C26 | -0.36 (16) |
| Ag1—O1—C1—C1 ⁱ | 160.03 (15) | C11—P1—C21—C26 | -111.04 (14) |
| N2—N1—C1—O1 | 5.0 (2) | Ag1—P1—C21—C26 | 126.88 (13) |
| N2—N1—C1—C1 ⁱ | -177.05 (14) | C31—P1—C21—C22 | -176.91 (12) |
| N1—N2—C2—C3 | 4.3 (2) | C11—P1—C21—C22 | 72.41 (13) |
| Ag1—N2—C2—C3 | -171.05 (12) | Ag1—P1—C21—C22 | -49.67 (13) |
| N1—N2—C2—C7 | 179.89 (13) | C26—C21—C22—C23 | 1.3 (2) |
| Ag1—N2—C2—C7 | 4.5 (2) | P1—C21—C22—C23 | 177.95 (13) |
| N2—C2—C3—C4 | 123.63 (18) | C21—C22—C23—C24 | -1.1 (3) |
| C7—C2—C3—C4 | -52.01 (19) | C22—C23—C24—C25 | 0.1 (3) |
| C2—C3—C4—C5 | 51.65 (19) | C23—C24—C25—C26 | 0.7 (3) |
| C3—C4—C5—C6 | -56.69 (19) | C22—C21—C26—C25 | -0.5 (3) |
| C4—C5—C6—C7 | 58.54 (18) | P1—C21—C26—C25 | -176.97 (14) |
| N2—C2—C7—C6 | -121.04 (16) | C24—C25—C26—C21 | -0.5 (3) |
| C3—C2—C7—C6 | 55.07 (19) | C21—P1—C31—C32 | -95.87 (14) |
| C5—C6—C7—C2 | -56.55 (18) | C11—P1—C31—C32 | 15.37 (15) |
| C21—P1—C11—C16 | 17.38 (16) | Ag1—P1—C31—C32 | 137.74 (12) |
| C31—P1—C11—C16 | -93.57 (15) | C21—P1—C31—C36 | 85.04 (14) |

| | | | |
|-----------------|--------------|-----------------|--------------|
| Ag1—P1—C11—C16 | 141.31 (13) | C11—P1—C31—C36 | -163.72 (13) |
| C21—P1—C11—C12 | -162.09 (12) | Ag1—P1—C31—C36 | -41.35 (15) |
| C31—P1—C11—C12 | 86.96 (13) | C36—C31—C32—C33 | 1.6 (3) |
| Ag1—P1—C11—C12 | -38.16 (13) | P1—C31—C32—C33 | -177.50 (14) |
| C16—C11—C12—C13 | 0.6 (2) | C31—C32—C33—C34 | -0.4 (3) |
| P1—C11—C12—C13 | -179.91 (13) | C32—C33—C34—C35 | -1.1 (3) |
| C11—C12—C13—C14 | -0.2 (3) | C33—C34—C35—C36 | 1.5 (3) |
| C12—C13—C14—C15 | -0.3 (3) | C34—C35—C36—C31 | -0.3 (3) |
| C13—C14—C15—C16 | 0.5 (3) | C32—C31—C36—C35 | -1.2 (3) |
| C14—C15—C16—C11 | -0.1 (3) | P1—C31—C36—C35 | 177.89 (16) |

Symmetry code: (i) $-x+1, -y+2, -z$.

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O2—H2A \cdots O3 | 0.80 | 2.02 | 2.8103 (17) | 167 |
| O2—H2B \cdots O3 ⁱⁱ | 0.88 | 1.98 | 2.8684 (16) | 177 |
| N1—H1 \cdots O5 ⁱⁱ | 0.88 | 2.16 | 2.8407 (19) | 134 |
| C22—H22 \cdots O4 | 0.95 | 2.58 | 3.297 (2) | 133 |

Symmetry code: (ii) $-x+1, -y+1, -z$.